



chain nodes :

1 2 3

ring nodes :

7 8 9 10 11 12 13 14 15 16 17 18

chain bonds :

1-3 1-2 1-11 2-14

ring bonds :

7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16 16-17 17-18

exact/norm bonds :

1-3 1-2 1-11 2-14 13-14 13-18 14-15 15-16 16-17 17-18

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12

G1:O,S

G2:C,N

G3:Cb,Cy,Hy

Match level :

1:CLASS 2:CLASS 3:CLASS 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS 12:CLASS 13:Atom
14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom